



Formula: C₁₅H₁₆O₉

MW: 340.29

Salt: H₂O

CAS: 531-75-9

TNP NUMBER: TNP00128

MDL NUMBER: MFCD00066712

IUPAC: 7-hydroxy-6-[3,4,5-trihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-2-yl oxy)]chromen-2-one

Smiles: O1C(C(C(C(O)C1CO)O)O)Oc1c(cc2oc(=O)ccc2c1)O

THERAPEUTIC CATEGORY: Skin Protectant

ACCEPTORS: 9

DONORS: 5

ROTATION BONDS: 8

N+O: 9

Chiral Centers: 5

LogP: -2.65

LogS: -2.24

LIPINSKI: 4

